Tinker 软件使用指南

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1. 软件介绍

A complete package for molecular mechanics, dynamics and modeling of molecules, especially biomacromolecules. TINKER has the ability to use any of several common parameter sets, such as Amber (ff94, ff96, ff98, ff99), CHARMM (19 and 27), Allinger MM (MM2-1991 and MM3-2000), OPLS (OPLS-UA, OPLS-AA and OPLS-AA/L), as well as the Jay Ponder Lab's own AMOEBA polarizable atomic multipole force field. TINKER implements a variety of novel algorithms including distance geometry with fast metrization and Gaussian trial distances, Elber's reaction path method, global optimization via their Potential Smoothing and Search algorithms, molecular dynamics with simulated annealing and stochastic dynamics options, particle mesh Ewald summation, Monte Carlo minimization, atomic multipole treatment of electrostatics with explicit dipole polarizability, Eisenberg-McLachlan ASP and GB/SA continuum solvation models, and truncated Newton TNCG local energy minimization.

2. 软件的安装与测试

安装方法

(refer to http://www.webmo.net/support/tinker.html)

% tar zxvf tinker.tar.gz

% cd /home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/

% cp make/Makefile source/
% cd source
% vim Makefile
% 修改 Makefile 中的

```
    TINKERDIR = /home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/
    BINDIR = /home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/bin
    LINKDIR = /usr/local/bin
    （uncomment the machine configuration parameters)
    Machine:  IntelPC / Linux
    CPU Type: Intel Xeon
    Oper Sys: Red Hat Linux
    Compiler: Intel Fortran
    (modify the parameters about the compiler)
    F77 = /home_soft/soft/x86_64/compiler/intel/11.0/081/bin/intel64/ifort
    LIBS =
    F77FLAGS = -c
```

```
    OPTFLAGS = -O2 -cm -w
    LIBFLAGS = -crusv
    LINKFLAGS = -Vaxlib

    % Make all
```

编译成功

```
5 cd ../
% mkdir bin
%cp –p source/*.x bin/
```

测试 % cd example %bin/analyze.x dialanine

2.1 安装目录及安装信息

源代码位置: /home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/source
安装后可运成程序的目录为：/home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/bin

2.2 测试结果

测试 1：

bench/bench1
串行运行
命令行：/home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/bin/timer.x bench1 N y
N：计算的参数规模

N	时间(s)
10	26s
100	265s
200	529s
500	1322s
1000	2646s

测试 2：

example/下所有用例，运行.run 文件即可，共有下列例子：
anion.run； cluster.run； cyclohex.run； enkephalin.run； helix.run；
argon.run； crambin.run； dialanine.run； formamide.run； salt.run

所有.run 文件中都有删除数据输出文件的 rm 语句，如想查看输出，则把相应语句注释即可

所有.run 文件中原来写的都是不带.x 的工具名称，已修正为*.x 的形式

3. 软件的运行使用方法

登录到 LB 结点之后，在$HOME/.bashrc 文件里面加入下面内容：
export PATH=$PATH:/home_soft/soft/x86_64/apps/OpenSoft/Chem/tinker/bin

进入数据所在目录，运行相应的文件即可